Alloy Design Workbench-Surface Modeling Package Developed

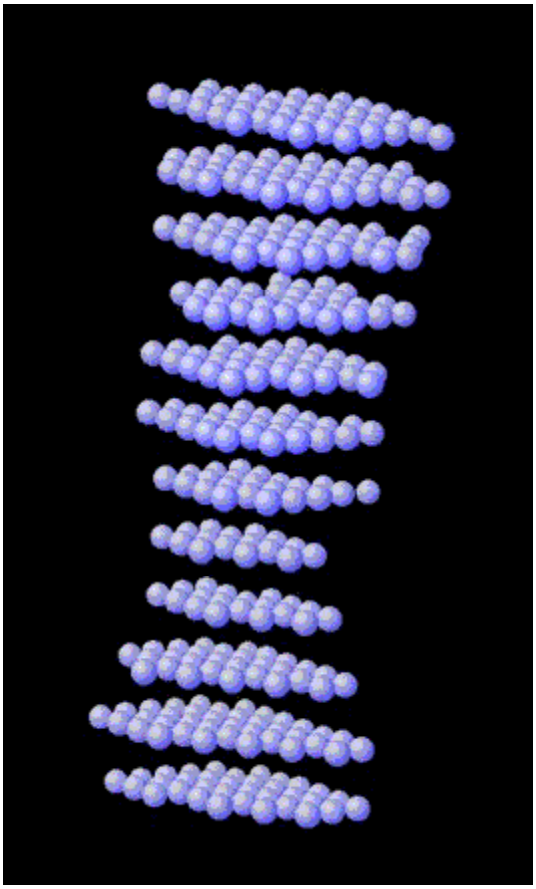
NASA Glenn Research Center’s Computational Materials Group has integrated a graphical user interface with in-house-developed surface modeling capabilities, with the goal of using computationally efficient atomistic simulations to aid the development of advanced aerospace materials, through the modeling of alloy surfaces, surface alloys, and segregation. The software is also ideal for modeling nanomaterials, since surface and interfacial effects can dominate material behavior and properties at this level. Through the combination of an accurate atomistic surface modeling methodology and an efficient computational engine, it is now possible to directly model these types of surface phenomenon and metallic nanostructures without a supercomputer.

Fulfilling a High Operating Temperature Propulsion Components (HOTPC) project level-I milestone, a graphical user interface was created for a suite of quantum approximate atomistic materials modeling Fortran programs developed at Glenn. The resulting "Alloy Design Workbench-Surface Modeling Package" (ADW-SMP) is the combination of proven quantum approximate Bozzolo-Ferrante-Smith (BFS) algorithms (refs. 1 and 2) with a productivity-enhancing graphical front end. Written in the portable, platform-independent Java programming language, the graphical user interface calls on extensively tested Fortran programs running in the background for the detailed computational tasks. Designed to run on desktop computers, the package has been deployed on PC, Mac, and SGI computer systems.

The graphical user interface integrates two modes of computational materials exploration. One mode uses Monte Carlo simulations to determine lowest energy equilibrium configurations. The second approach is an interactive "what if" comparison of atomic configuration energies, designed to provide real-time insight into the underlying drivers of alloying processes.

By using a Metropolis Monte Carlo algorithm for atomic exchanges, ADW-SMP can simulate an annealing run on an alloy, prompting the user for the number of temperature stages, the number of atomic exchanges per stage, and the temperature of each stage of the anneal. At each temperature, a Metropolis algorithm is used to determine if two unlike atoms in the alloy should be exchanged, considering whether the exchange lowers or raises the total energy of the material. Another option of particular importance for surfaces is a lattice position relaxation calculation, in which the coordinates of each atom can be optimized. Because they are located on the surface, atoms can rearrange to lower the total energy of the computational cell in a process called surface reconstruction, which can greatly affect subsequent surface interactions. The ADW-SMP program then gives the user a graphical representation of the results, as well as available statistical summaries such as the coordinatio n of each type of atom in the computational cell, indicating the type and number of neighboring atoms at nearest- and next-nearest-neighbor distances.

In the second approach to alloy modeling implemented in ADW-SMP, the static energies of similar collections of atoms are computed and compared. This allows users to explore how arranging atoms in different configurations affects the total energy. The ability to perform atom-by-atom analysis of the energetics helps users to understand most surface processes in greater detail. For example, users can learn why, energetically, specific alloy components may segregate preferentially to a surface, either promoting or poisoning catalytic reactions, or determine why some otherwise immiscible metals will form surface alloys, mixing only in the presence of a surface.



Display from the ADW-SMP of an annealed face-centered cubic [111] copper nanowire showing initial indications of local thinning.

This figure depicts an example computational cell, showing the real-time, three-dimensional representation of the array of atoms as seen by a user. Shown is an annealed copper nanowire with local thinning becoming visible. Extensive atom display routines enable on-screen manipulation to better visualize and understand the atomic arrangements and their energetically favored configurations, under interactive pointer control. Incorporated editing capabilities allow users to graphically choose atoms to move or modify or to choose where to place additional alloying components.

With the ever-increasing computational power available to researchers on their own desktops, more sophisticated simulation tools become increasingly attractive. For

materials scientists engaged in the creation of advanced alloys, the ADW-SMP software suite should become an interesting tool to potentially guide and instruct parallel experimental work. With immediate, on-screen feedback, researchers can design and launch alloy simulations to guide the much more expensive laboratory explorations of alloy properties, or use the simulations to aid in detailed interpretation of experimental results.

Find out more about this research http://www.icmsc.org/.

References

1. Bozzolo, G., et al.: An Introduction to the BFS Method and Its Use to Model Binary NiAl Alloys. J. Computer-Aided Mater. Design, vol. 6, no. 1, 1999, pp. 1-32.

2. Bozzolo, G., et al.: Surface Segregation in Multicomponent Systems: Modeling of Surface Alloys and Alloy Surfaces. Comput. Mater. Sci., vol. 15, no. 2, 1999, pp. 169-195.

Glenn contacts: Dr. Phillip B. Abel, 216-433-6063, Phillip.B.Abel@nasa.gov; and Dr. Ronald D. Noebe, 216-433-2093, Ronald.D.Noebe@nasa.gov

Ohio Aerospace Institute (OAI) contact: Dr. Guillermo Bozzolo, 440-962-3103, Guillermo.H.Bozzolo@grc.nasa.gov
Authors: Dr. Phillip B. Abel, Dr. Ronald D. Noebe, Dr. Guillermo H. Bozzolo, Dr. Brian S. Good, and Elaine S. Daugherty

Headquarters program office: OAT
Programs/Projects: Propulsion and Power, HOTPC